

University of Groningen

Interaction dynamics in collisions of ions with molecules and clusters

Postma, Jos Jacob Uilke

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version

Publisher's PDF, also known as Version of record

Publication date:

2011

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Postma, J. J. U. (2011). *Interaction dynamics in collisions of ions with molecules and clusters*. s.n.

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Interaction Dynamics in Collisions of Ions with Molecules and Clusters

COVER: *A rendering of a recoil ion momentum spectrometer.*



PRINTED BY: Ipskamp Drukkers, Enschede, June 2011.

RIJKSUNIVERSITEIT GRONINGEN

Interaction Dynamics in Collisions of Ions with Molecules and Clusters

Proefschrift

ter verkrijging van het doctoraat in de
Wiskunde en Natuurwetenschappen
aan de Rijksuniversiteit Groningen
op gezag van de
Rector Magnificus, dr. E. Sterken,
in het openbaar te verdedigen op
vrijdag 15 juli 2011
om 16:15 uur

door

Jos Jacob Ulke Postma

geboren op 27 april 1982
te Engwierum

Promotor : Prof. dr. ir. R. A. Hoekstra

Copromotor : Dr. T. A. Schlathölder

Beoordelingscommissie : Prof. dr. J. Oomens
Prof. dr. A.G.G.M. Tielens
Prof. dr. R.G.E. Timmermans

ISBN (Gedrukte versie) : 978-90-367-4979-4

ISBN (Elektronische versie) : 978-90-367-4980-0

Contents

1	Introduction	1
1.1	General Introduction	1
1.2	PAH Molecules in Interstellar Space	2
1.3	Measurement of Processes in Atomic Systems	4
1.4	Thesis Outline	6
2	Experimental Setup and Techniques	7
2.1	Introduction	7
2.2	ECR Ion Source and Ion Beam Transport	7
2.3	Setup	8
2.4	Time-of-Flight Mass Spectrometry	9
2.4.1	Linear Time-of-Flight Spectrometer	9
2.4.2	Reflectron Time-of-Flight Spectrometer	11
2.5	Ion Beam Chopping	14
2.6	Data Acquisition	16
2.7	Transmission	19
3	Interactions of Anthracene with keV Light Ions	23
3.1	Introduction	23
3.2	Experiment	24
3.3	Fragment Mass Spectra	25
3.4	Discussion	29
3.4.1	Electronic Stopping	34
3.5	Astronomical Implications	40
3.6	Conclusion	41
4	Ion-PAH sub-keV Interactions	43
4.1	Introduction	43
4.2	Theory of Molecular Bonding and Collisions	44
4.2.1	Introduction	44

4.2.2	Abell-Tersoff	44
4.2.3	Tersoff-Brenner	46
4.2.4	Modeling of Fast Particle (Screened-)Coulomb Interactions	49
4.3	Molecular Dynamics Simulations	50
4.3.1	Introduction	50
4.3.2	Potential Derivatives	50
4.3.3	Finite Difference Integration Schemes	52
4.4	Results and Discussion	54
4.4.1	Molecular Dynamics: Setup and Validation	54
4.4.2	Results for H and He Colliding with Anthracene: Direct Fragmentation	56
4.4.3	Monte Carlo Simulations: Cross Sections	66
4.4.4	Dissociation	68
4.5	Conclusions	72
5	Towards RIMS of Molecules and Clusters	75
5.1	Introduction	75
5.2	Basics of Supersonic Jet Production	76
5.2.1	Classical Nucleation Theory	76
5.2.2	Supersonic Expansion: Molecular Beam Source	78
5.2.3	Cluster Formation in Supersonic Expansions	79
5.2.4	Properties of Jet Expansions	82
5.3	Characterization of Ar Cluster Beams by Ion Impact	87
5.3.1	Setup for Characterization of Cluster Jets	87
5.3.2	Fragment Mass Spectra	87
5.3.3	Kinetic Energy Releases	93
5.4	Recoil Ion Momentum Spectrometry	96
5.4.1	Momentum Reconstruction in the Laboratory Frame	99
5.4.2	Momentum Reconstruction in the Center of Mass Frame	100
5.4.3	CRIMS Setup and Characterization	103
5.5	Conclusions	110
6	Summary and Outlook	111
6.1	Summary	111
6.2	Outlook	113
A	Atomic Units	115
B	Bicubic and Tricubic Interpolation	117
B.1	Bicubic Interpolation	117
B.2	Tricubic Interpolation	120
	List of Acronyms and Abbreviations	123
	Samenvatting	125

Dankwoord	129
------------------	------------

Bibliography	131
---------------------	------------

